

FILE 'CASREACT' ENTERED AT 17:52:11 ON 12 JUN 2007
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

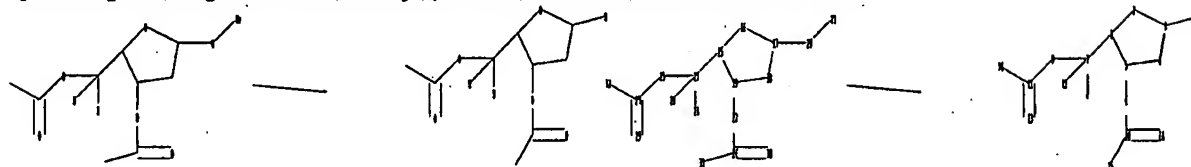
New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 12 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database, compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction VI to I.str



chain nodes :
6 7 8 9 10 11 12 13 14 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35
ring nodes :
1 2 3 4 5 15 16 17 18 19
chain bonds :
1-7 3-31 5-6 6-10 7-8 7-9 7-12 9-11 10-14 10-35 11-13 11-34 15-23 17-20 19-22 20-21
22-26 23-24 23-25 23-28 25-27 26-30 26-33 27-29 27-32
ring bonds :
1-2 1-5 2-3 3-4 4-5 15-16 15-19 16-17 17-18 18-19
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-10 7-9 9-11 10-14 11-13 15-16 15-19 16-17 17-18 17-20 18-19
19-22 22-26 23-25 25-27 26-30 27-29
exact bonds :
1-7 3-31 7-8 7-12 10-35 11-34 15-23 20-21 23-24 23-28 26-33 27-32

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS
34:CLASS 35:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 15

L1 STRUCTURE UPLOADED

=> s 11
SAMPLE SEARCH INITIATED 17:52:40 FILE 'CASREACT'
SCREENING COMPLETE - 1 REACTIONS TO VERIFY FROM 1 DOCUMENTS
100.0% DONE 1 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 1 TO 79
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 17:52:43 FILE 'CASREACT'
SCREENING COMPLETE - 144 REACTIONS TO VERIFY FROM 86 DOCUMENTS

100.0% DONE 144 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1 (0 REACTIONS)

=> file stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	113.55	113.76

FILE 'STNGUIDE' ENTERED AT 17:52:52 ON 12 JUN 2007
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 8, 2007 (20070608/UP).

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.12	113.88

FILE 'CASREACT' ENTERED AT 17:53:48 ON 12 JUN 2007
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

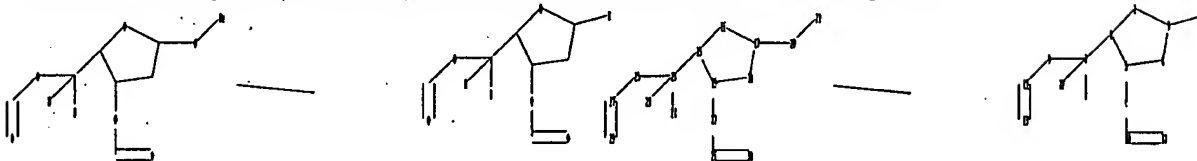
* CASREACT now has more than 12 million reactions *
* *****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

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=>

Uploading C:\Program Files\Stnexp\Queries\10578800\reaction VI to I acyl.str



chain nodes :
6 7 8 9 10 11 12 13 14 20 21 22 23 24 25 26 27 28 29 30 31
ring nodes :
1 2 3 4 5 15 16 17 18 19
chain bonds :
1-7 3-31 5-6 6-10 7-8 7-9 7-12 9-11 10-14 11-13 15-23 17-20 19-22 20-21 22-26 23-24
23-25 23-28 25-27 26-30 27-29

ring bonds :
 1-2 1-5 2-3 3-4 4-5 15-16 15-19 16-17 17-18 18-19
 exact/norm bonds :
 1-2 1-5 2-3 3-4 4-5 5-6 6-10 7-9 9-11 10-14 11-13 15-16 15-19 16-17 17-18 17-20 18-19
 19-22 22-26 23-25 25-27 26-30 27-29
 exact bonds :
 1-7 3-31 7-8 7-12 15-23 20-21 23-24 23-28

Match level :
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 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS
 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

L4 STRUCTURE UPLOADED

=> d
 L4 HAS NO ANSWERS
 L4 STR
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l4
 SAMPLE SEARCH INITIATED 17:54:10 FILE 'CASREACT'
 SCREENING COMPLETE - 70 REACTIONS TO VERIFY FROM 18 DOCUMENTS
 100.0% DONE 70 VERIFIED 0 HIT RXNS 0 DOCS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED VERIFICATIONS: 899 TO 1901
 PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4 (0 REACTIONS)

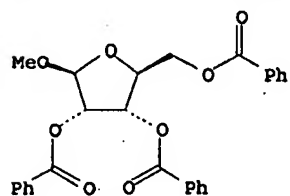
=> s l4 full
 FULL SEARCH INITIATED 17:54:13 FILE 'CASREACT'
 SCREENING COMPLETE - 4637 REACTIONS TO VERIFY FROM 461 DOCUMENTS
 100.0% DONE 4637 VERIFIED 64 HIT RXNS 28 DOCS
 SEARCH TIME: 00.00.01

L6 28 SEA SSS FUL L4 (.64 REACTIONS)

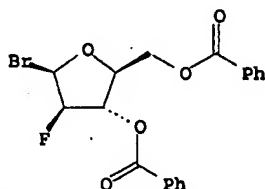
=> d l6 1-28

L6 ANSWER 1 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(86) OF 183 - 5 STEPS



1. Ac2O, H2SO4, Water, AcOH
2. HBr, Water, CH2Cl2
- 3.1. SO2Cl2, CH2Cl2, DMF
- 3.2. 1H-Imidazole
4. KHF2, HF, S:123513-85-9, Water
5. HBr, AcOH, CH2Cl2

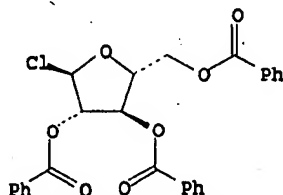
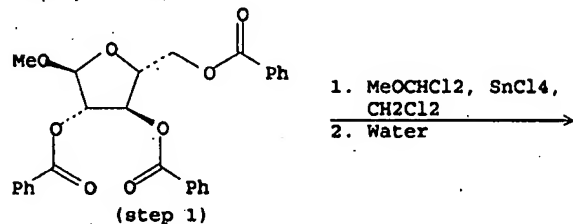


REF: Faming Zhuanli Shengqing Gongkai Shuomingshu, 1891710, 10 Jan 2007

NOTE: 2) regioselective, 4) stereoselective, 5) regioselective, in the dark
 CON: STEP(1.1) 0 deg C; 0 deg C -> room temperature; overnight, cooled
 STEP(2.1) 3.5 hours, 0 deg C; 2 hours, room temperature
 STEP(3.1) -15 deg C; 0.5 hours, -15 deg C;
 -15 deg C -> room temperature; 4 hours, room temperature
 STEP(3.2) 0 deg C; 17 hours, room temperature
 STEP(4.1) room temperature -> 150 deg C; 150 deg C -> 160 deg C;
 1 hour, 160 deg C
 STEP(5) 24 hours, room temperature

L6 ANSWER 2 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(35) OF 806



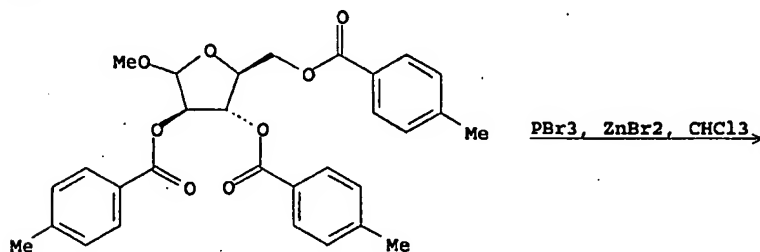
REF: Journal of Organic Chemistry, 71(21), 8071-8088; 2006

NOTE: regioselective

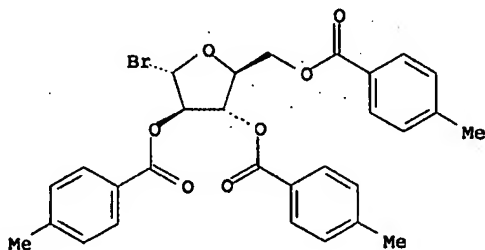
CON: STAGE(1) 13 hours, room temperature
 STAGE(2) 45 minutes, room temperature

L6 ANSWER 3 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 17



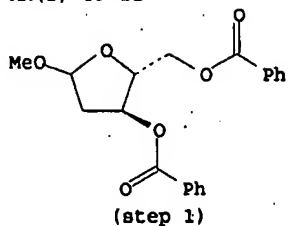
RX(1) OF 17



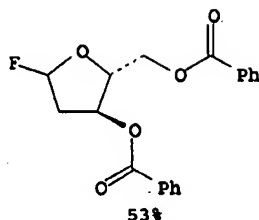
488

REF: Eur. Pat. Appl., 1705181, 27 Sep 2006
 CON: 19 hours, 45 deg C

RX(2) OF 21



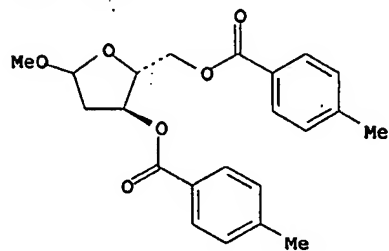
1. HCl, Water,
Dioxane
2. DAST [(Et2N).SF3],
THF
3. MeOH



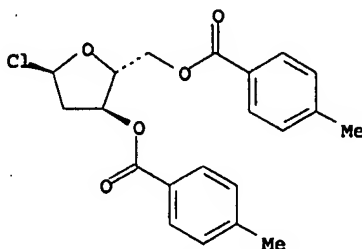
REF: Journal of the American Chemical Society, 127(44), 15612-15617;
2005

CON: STAGE(1) 1 hour, reflux
STAGE(2) -78 deg C; 20 minutes, room temperature
STAGE(3) room temperature

RX(2) OF 33



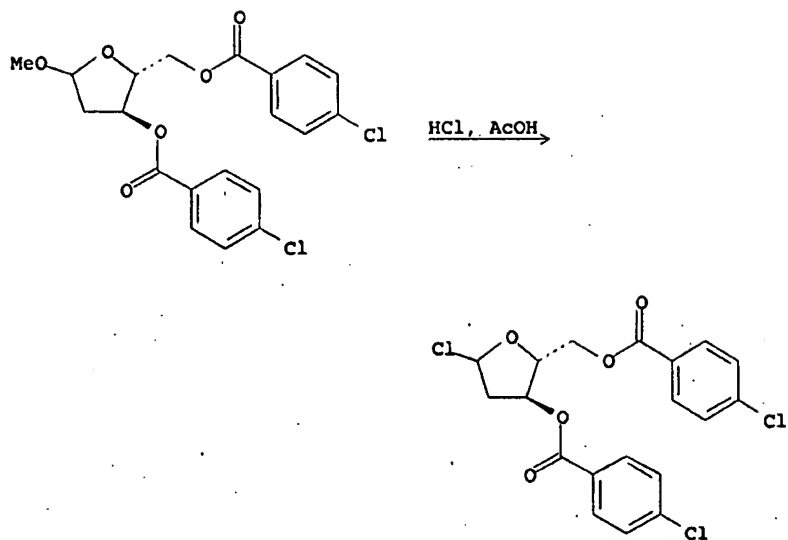
HCl, Et2O



REF: Organic Letters, 7(14), 2853-2856; 2005

NOTE: stereoselective
CON: 10 minutes, 0 deg C

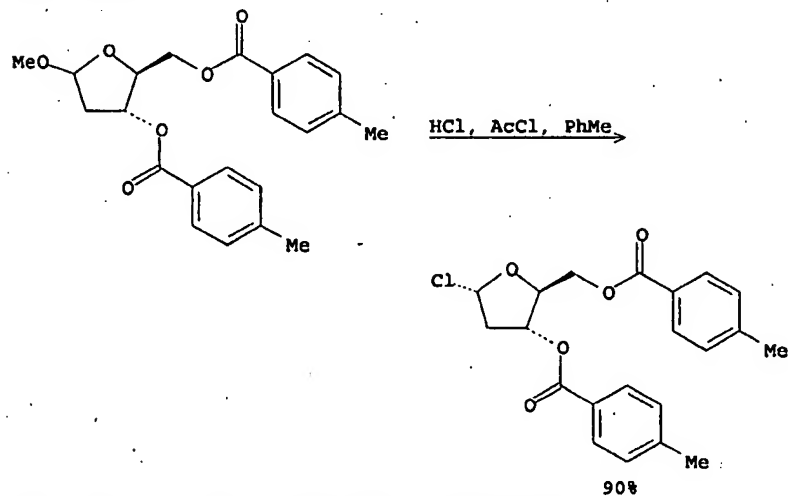
RX(4) OF 21



REF: Faming Zhuanli Shengqing Gongkai Shuomingshu, 1539845, 27 Oct 2004
CON: 2 - 4 hours, 30 deg C

L6 ANSWER 7 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(6) OF 24

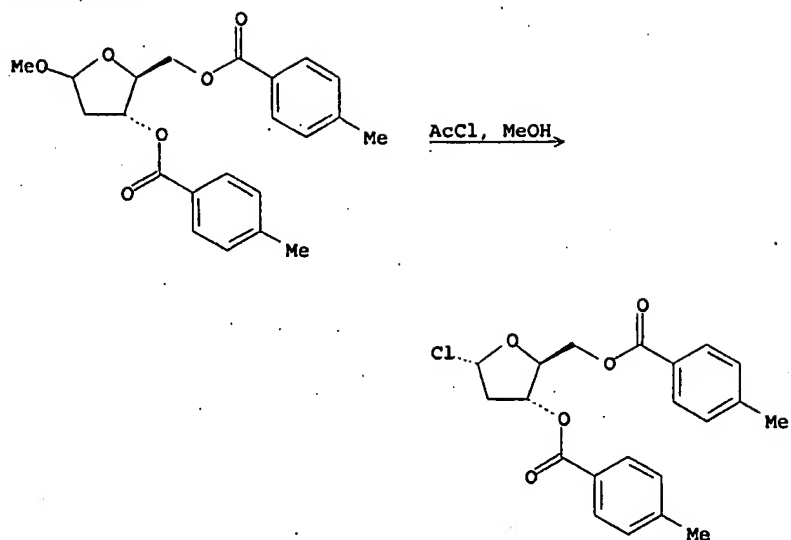


REF: PCT Int. Appl., 2005044832, 19 May 2005

CON: STAGE(1) room temperature; room temperature -> 5 deg C;
<15 deg C; 1 hour, 5 deg C

L6 ANSWER 8 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 32



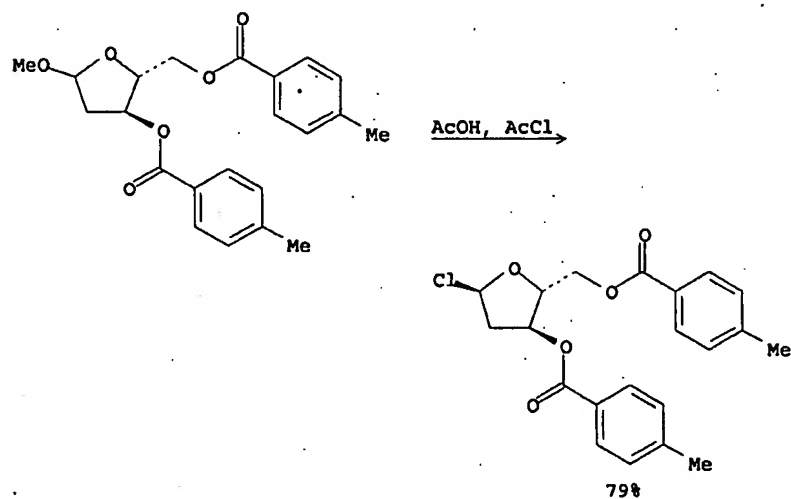
REF: U.S. Pat. Appl. Publ., 2004266996, 30 Dec 2004

NOTE: workup

CON: STAGE(1) room temperature; room temperature \rightarrow 10 deg C;
3.5 - 4 hours, 8 - 10 deg C; 4 hours, 8 - 10 deg C

L6 ANSWER 9 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 64



79%

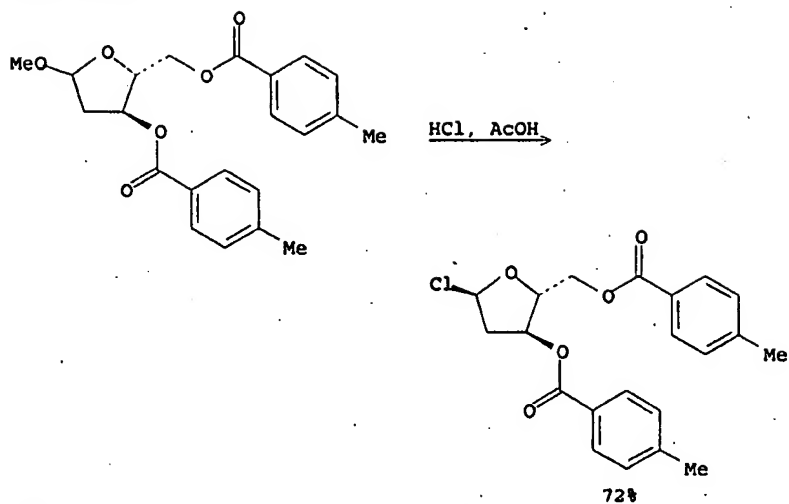
REF: Organic & Biomolecular Chemistry, 1(13), 2267-2275; 2003

NOTE: stereoselective

CON: room temperature

L6 ANSWER 10 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(4) OF 34

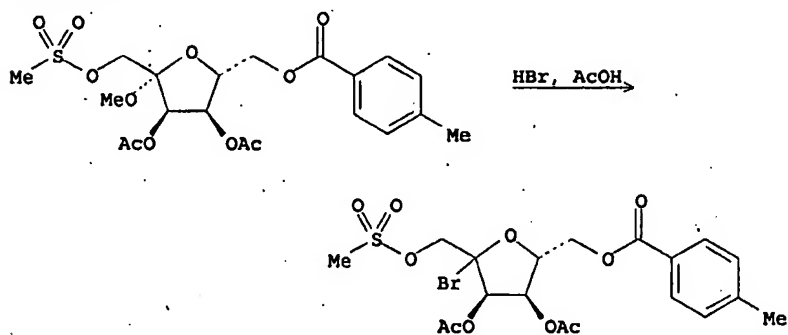


REF: Organic Letters, 4(26), 4571-4574; 2002

CON: STAGE(1) 5 minutes, room temperature; 1 hour, 10 deg C

L6 ANSWER 11 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(10) OF 74

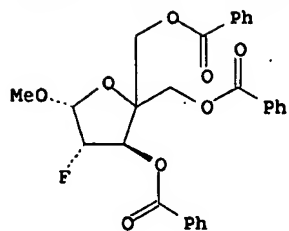


REF: Tetrahedron Letters, 43(37), 6553-6555; 2002

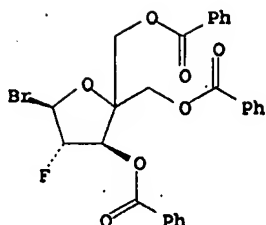
CON: 1 - 3 hour, 20 deg C

L6 ANSWER 12 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(57) OF 206 - 3 STEPS



1. F3CCO2H, Water
2. Ac2O, Pyridine
3. HBr, AcOH

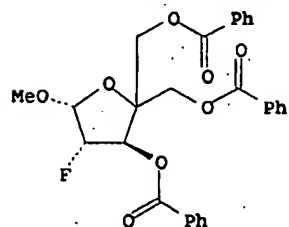


REF: Nucleosides, Nucleotides & Nucleic Acids, 20(4-7), 747-750; 2001

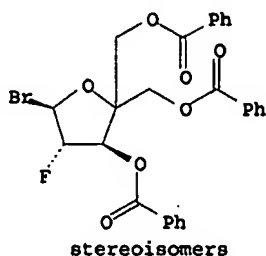
NOTE: 1) stereoselective, 2:1 alpha:beta, 2) stereoselective, 3:1 alpha:beta, 3) stereoselective, 6:1 alpha:beta

L6 ANSWER 13 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(62) OF 180 - 3 STEPS



1.1. F3CCO2H, Water
1.2. NaHCO3, Water
2. Ac2O, Pyridine
3. HBr, CH2Cl2, AcOH

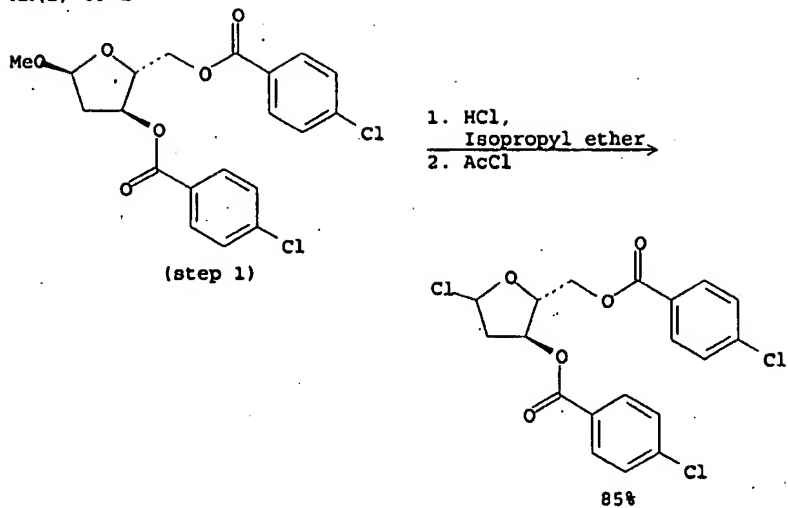


REF: Nucleosides, Nucleotides & Nucleic Acids, 20(8), 1583-1598; 2001

NOTE: 1) 67:33 alpha:beta, stereoselective, 2) stereoselective, 3) 86:14 alpha:beta, stereoselective

L6 ANSWER 14 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

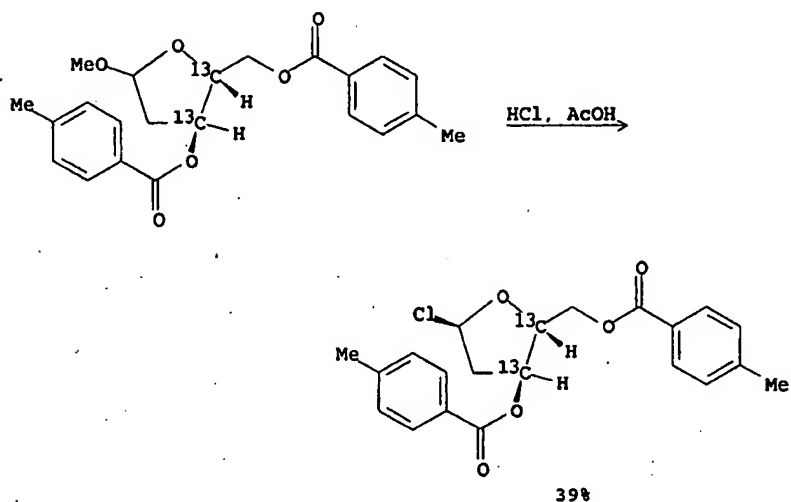
RX(1) OF 1



REF: Jpn. Kokai Tokkyo Koho, 2000290289, 17 Oct 2000

L6 ANSWER 15 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(10) OF 66



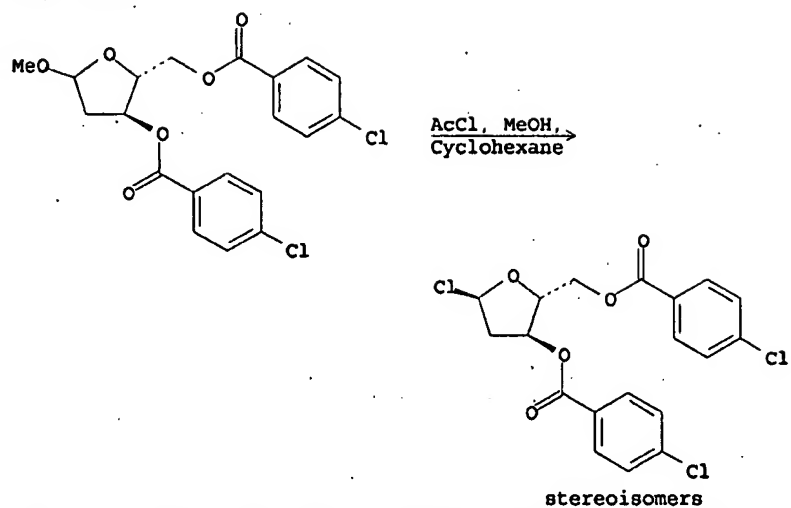
REF: European Journal of Organic Chemistry, (5), 861-866; 2000

NOTE: gaseous HCl used

CON: STAGE(1) 0 deg C; 10 minutes

L6 ANSWER 16 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 8

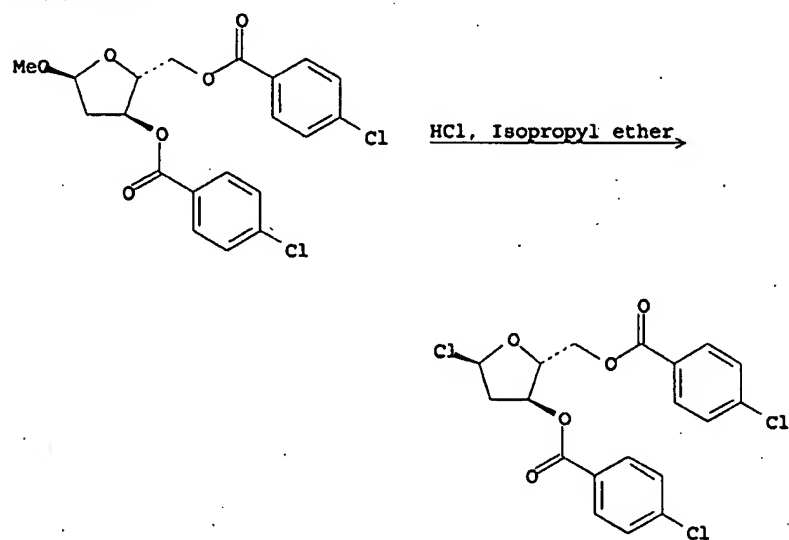


REF: Jpn. Kokai Tokkyo Koho, 07224081, 22 Aug 1995, Heisei

NOTE: 25.degree. for 4 h; 84.8% yield

L6 ANSWER 17 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

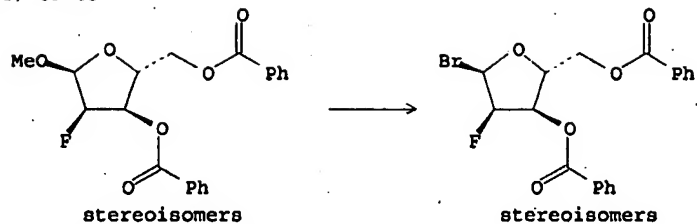
RX(7) OF 28



REF: Eur. Pat. Appl., 635517, 25 Jan 1995

L6 ANSWER 18 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

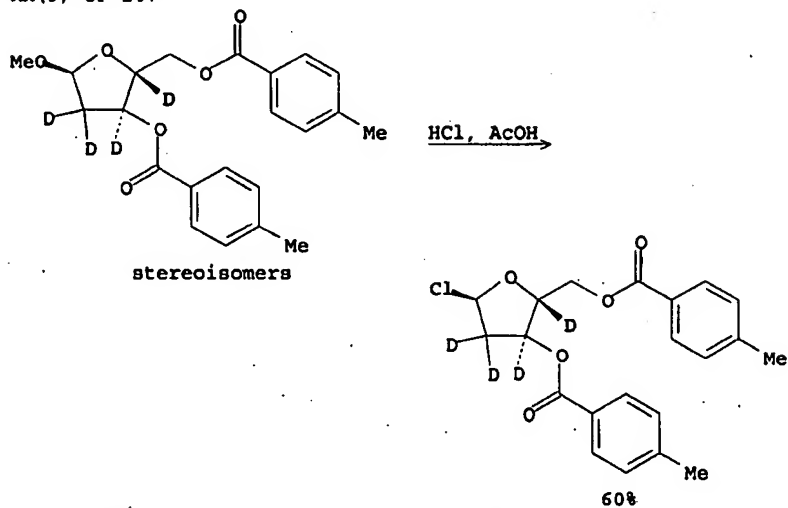
RX(1) OF 83



REF: PCT Int. Appl., 9310137, 27 May 1993
NOTE: 2 STEPS

L6 ANSWER 19 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

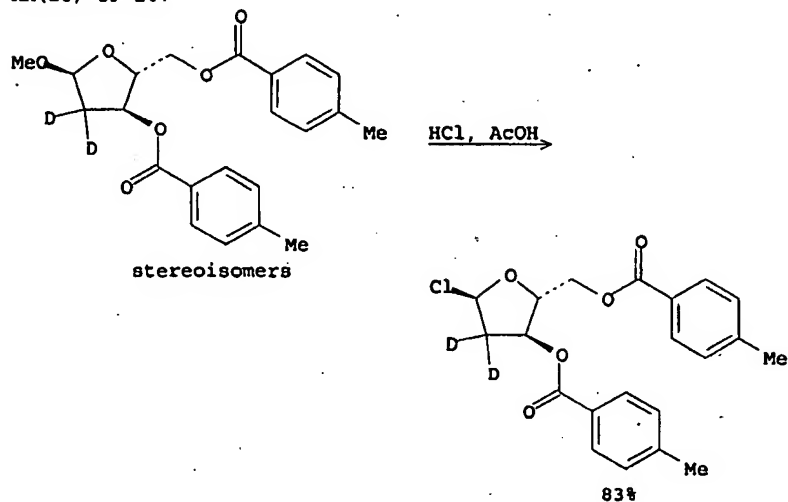
RX(9) OF 147



REF: Tetrahedron, 43(18), 4227-34; 1987

L6 ANSWER 20 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

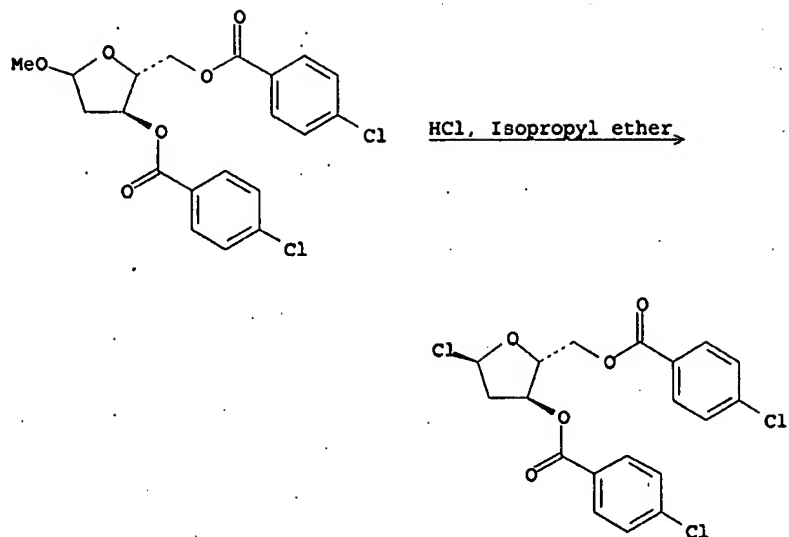
RX(18) OF 147



REF: Tetrahedron, 43(10), 2355-68; 1987

L6 ANSWER 21 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

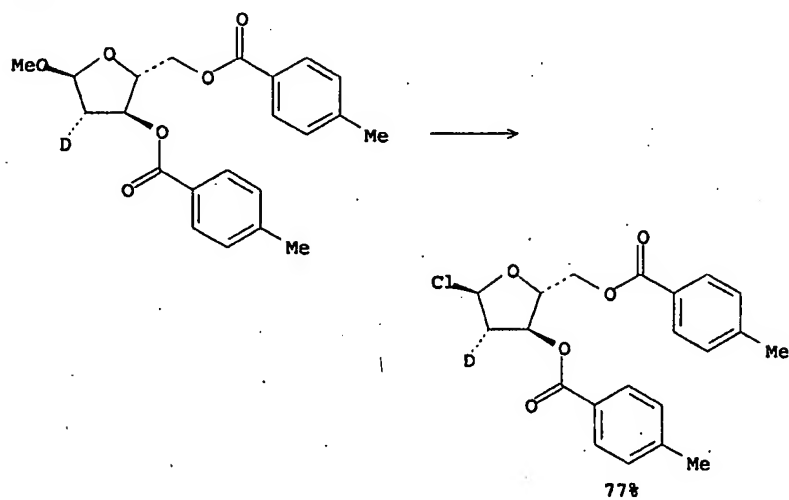
RX(2) OF 88



REF: Nippon Kagaku Kaishi, (12), 1765-70; 1986

L6 ANSWER 22 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

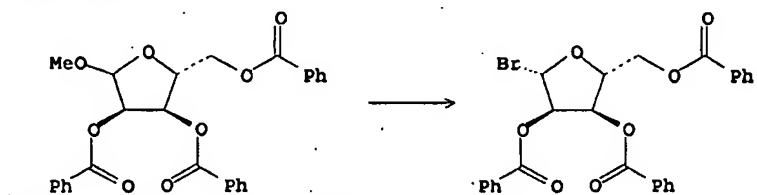
RX(6) OF 177



REF: Tetrahedron, 42(19), 5427-41; 1986

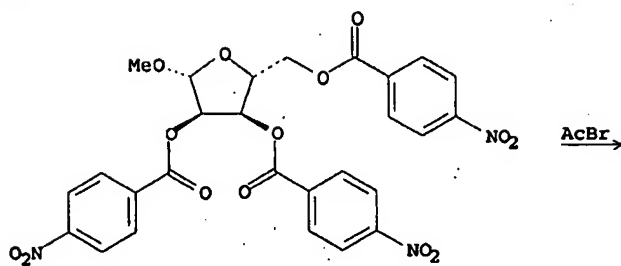
L6 ANSWER 23 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 5

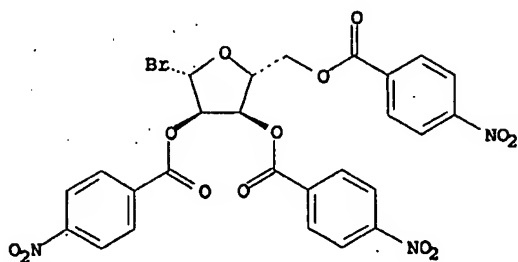


REF: Eur. Pat. Appl., 145978, 26 Jun 1985

RX(2) OF 3

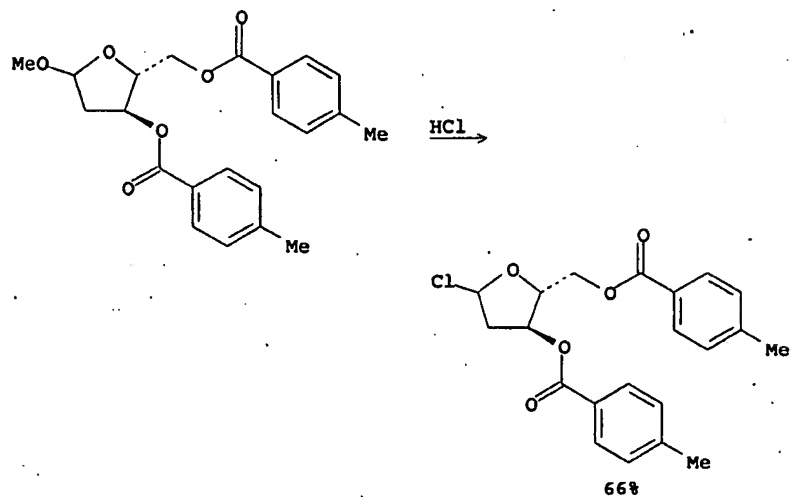


RX(2) OF 3



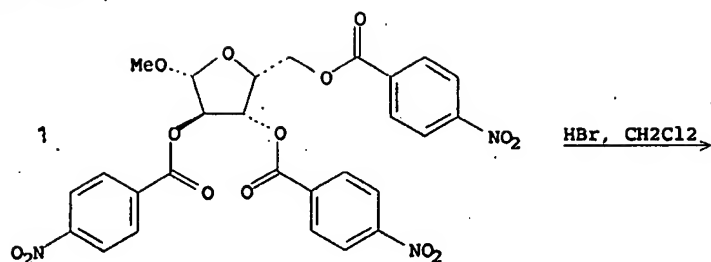
REF: U.S., 4282349, 04 Aug 1981

RX(1) OF 51

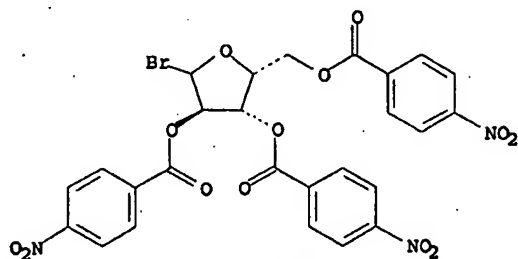


REF: U.S., 4239753, 16 Dec 1980

RX(1) OF 1



RX(1) OF 1



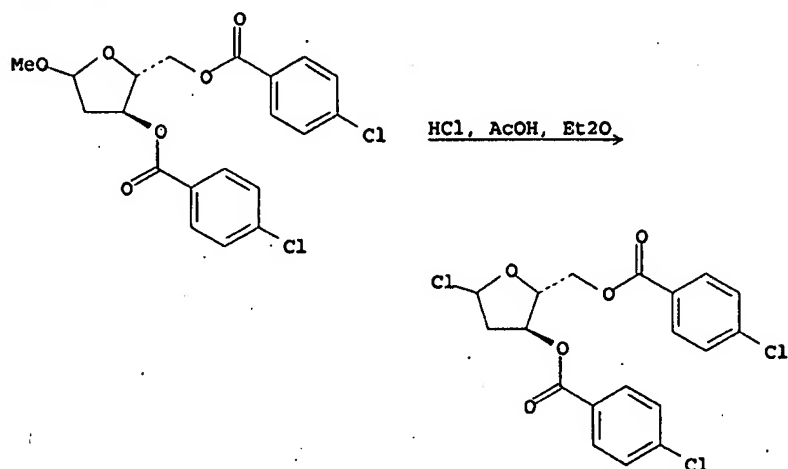
68%

REF: Carbohydrate Research, 47(2), 233-40; 1976

NOTE: Classification: Substitution; Bromination; # Conditions: HBr
CH₂Cl₂; 24h 0-3 deg

L6 ANSWER 27 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 13



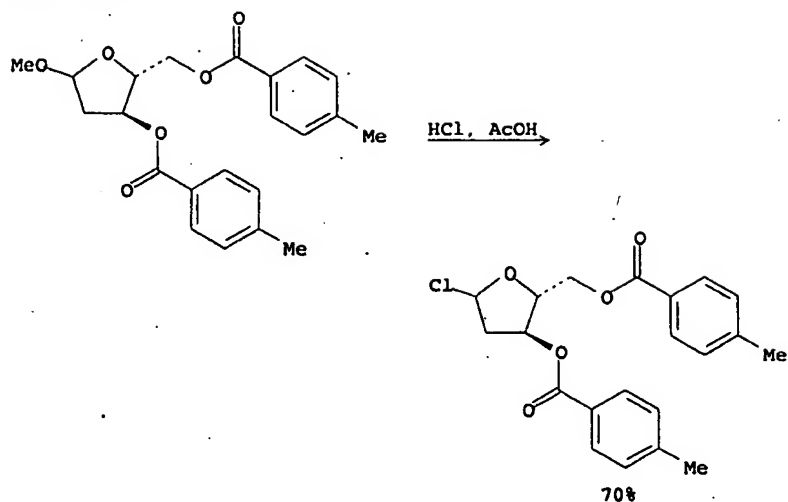
65%

REF: Journal of the American Chemical Society, 83,, 4066-50; 1961

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl
Et₂O AcOH

L6 ANSWER 28 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3



REF: Journal of the American Chemical Society, 81,, 4112-13; 1959

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl
AcOH

=> d his

(FILE 'HOME' ENTERED AT 17:52:00 ON 12 JUN 2007)

FILE 'CASREACT' ENTERED AT 17:52:11 ON 12 JUN 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 0 S L1 FULL

FILE 'STNGUIDE' ENTERED AT 17:52:52 ON 12 JUN 2007

FILE 'CASREACT' ENTERED AT 17:53:48 ON 12 JUN 2007
L4 STRUCTURE UPLOADED
L5 0 S L4
L6 28 S L4 FULL

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE
ENTRY
194.08

TOTAL
SESSION
307.96

STN INTERNATIONAL LOGOFF AT 17:54:44 ON 12 JUN 2007

FILE 'CASREACT' ENTERED AT 17:59:12 ON 12 JUN 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

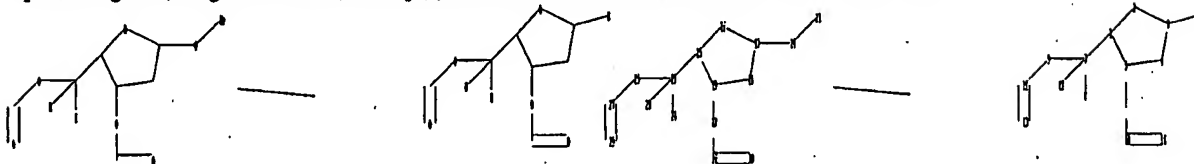
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chain nodes :
6 7 8 9 10 11 12 13 14 20 21 22 23 24 25 26 27 28 29 30 31
ring nodes :
1 2 3 4 5 15 16 17 18 19
chain bonds :
1-7 3-31 5-6 6-10 7-8 7-9 7-12 9-11 10-14 11-13 15-23 17-20 19-22 20-21 22-26 23-24
23-25 23-28 25-27 26-30 27-29
ring bonds :
1-2 1-5 2-3 3-4 4-5 15-16 15-19 16-17 17-18 18-19
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-10 7-9 9-11 10-14 11-13 15-16 15-19 16-17 17-18 17-20 18-19
19-22 22-26 23-25 25-27 26-30 27-29
exact bonds :
1-7 3-31 7-8 7-12 15-23 20-21 23-24 23-28

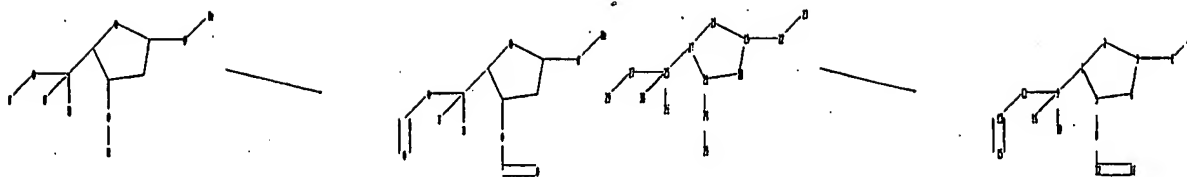
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

L1 STRUCTURE UPLOADED

=> s ll full
FULL SEARCH INITIATED 17:59:29 FILE 'CASREACT'
SCREENING COMPLETE : 4637 REACTIONS TO VERIFY FROM 461 DOCUMENTS
100.0% DONE 4637 VERIFIED 64 HIT RXNS 28 DOCS
SEARCH TIME: 00.00.01

L2 28 SEA SSS FUL L1 (64 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction V to VI.str



chain nodes :
 6 7 8 9 10 11 12 13 14 15 16 22 23 24 25 26 27 28 29 30
 ring nodes :
 1 2 3 4 5 17 18 19 20 21
 chain bonds :
 1-9 3-6 5-8 6-7 8-12 9-10 9-11 9-14 11-13 12-16 13-15 17-25 19-22 21-24 22-23 24-28
 25-26 25-27 25-30 27-29
 ring bonds :
 1-2 1-5 2-3 3-4 4-5 17-18 17-21 18-19 19-20 20-21
 exact/norm bonds :
 1-2 1-5 2-3 3-4 3-6 4-5 5-8 8-12 9-11 11-13 12-16 13-15 17-18 17-21 18-19 19-20 19-22
 20-21 21-24 25-27
 exact bonds :
 1-9 6-7 9-10 9-14 17-25 22-23 24-28 25-26 25-30 27-29

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS
 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
 fragments assigned product role:
 containing 1
 fragments assigned reactant/reagent role:
 containing 17

L3 STRUCTURE UPLOADED

=> s l3
 SAMPLE SEARCH INITIATED 17:59:52 FILE 'CASREACT'
 SCREENING COMPLETE - 581 REACTIONS TO VERIFY FROM 45 DOCUMENTS
 100.0% DONE 581 VERIFIED 2 HIT RXNS 2 DOCS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED VERIFICATIONS: 10175 TO 13065
 PROJECTED ANSWERS: 2 TO 124

L4 2 SEA SSS SAM L3 (2 REACTIONS)

=> s l3 full
 FULL SEARCH INITIATED 17:59:55 FILE 'CASREACT'
 SCREENING COMPLETE - 11450 REACTIONS TO VERIFY FROM 894 DOCUMENTS
 100.0% DONE 11450 VERIFIED 66 HIT RXNS 43 DOCS
 SEARCH TIME: 00.00.01

L5 43 SEA SSS FUL L3 (66 REACTIONS)

=> d his

(FILE 'HOME' ENTERED AT 17:59:06 ON 12 JUN 2007)

FILE 'CASREACT' ENTERED AT 17:59:12 ON 12 JUN 2007

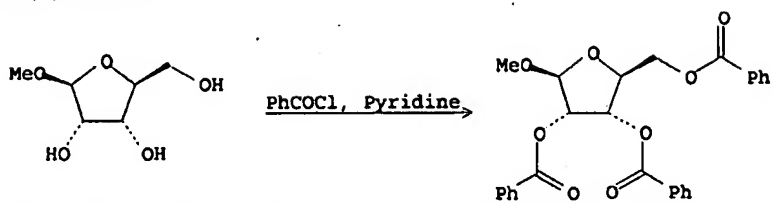
L1 STRUCTURE UPLOADED
 L2 28 S L1 FULL
 L3 STRUCTURE UPLOADED
 L4 2 S L3
 L5 43 S L3 FULL

=> s l2 and l5
 L6 13 L2 AND L5

=> d 16 1-13

L6 ANSWER 1 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 183

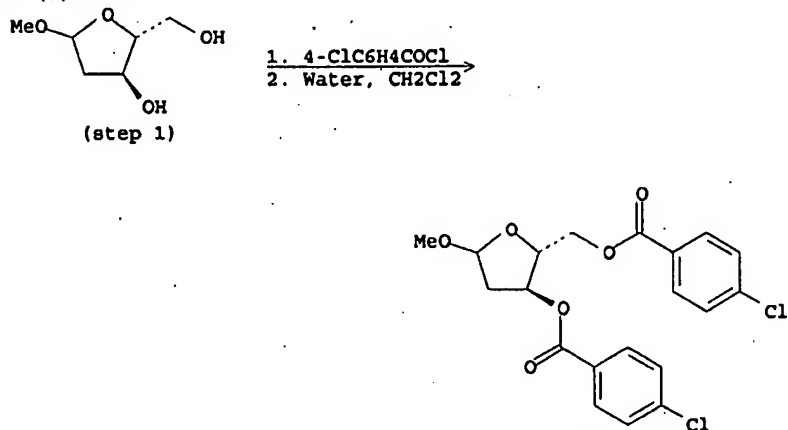


REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1891710, 10 Jan 2007

CON: STAGE(1) 0 deg C; 17 hours, room temperature

L6 ANSWER 2 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 21

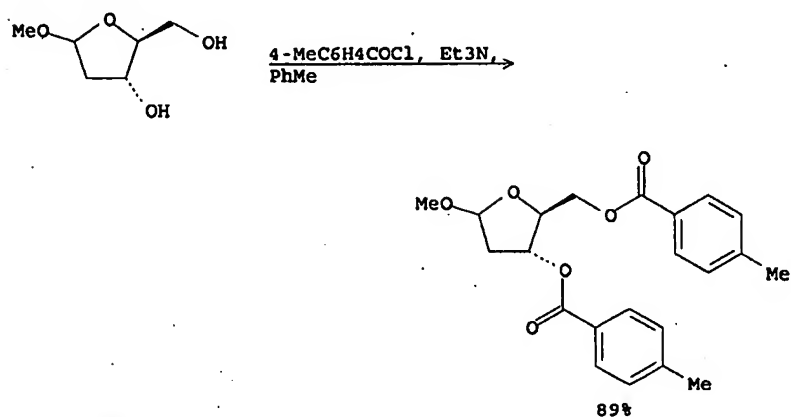


REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1539845, 27 Oct 2004

CON: STAGE(1) 4 - 5 hours, 40 deg C
STAGE(2) 0.5 hours, 5 - 10 deg C

L6 ANSWER 3 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(4) OF 24



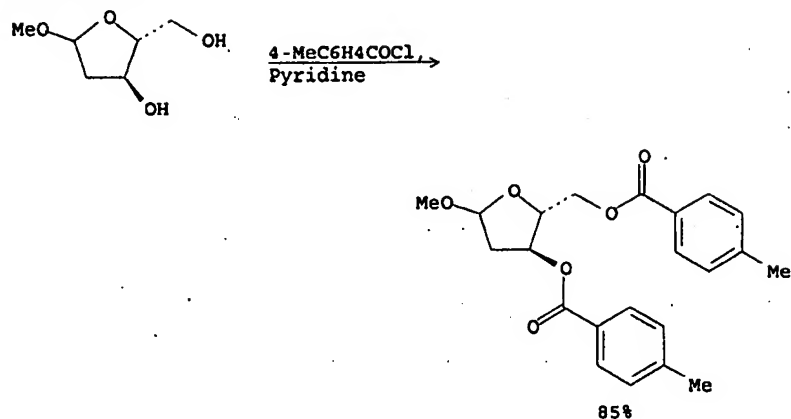
89%

REF: PCT Int. Appl., 2005044832, 19 May 2005

CON: STAGE(1) room temperature -> 40 deg C; 40 deg C -> 60 deg C;
5 hours, 60 deg C

L6 ANSWER 4 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

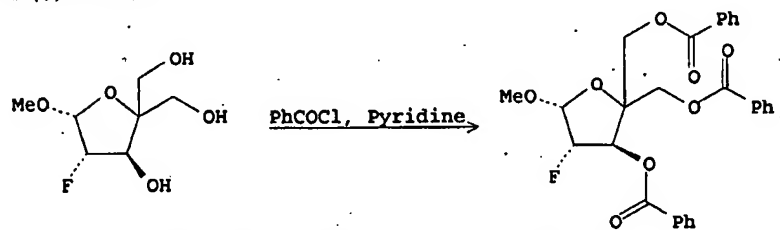
RX(2) OF 34



REF: Organic Letters, 4(26), 4571-4574; 2002
CON: STAGE(1) 0 deg C; overnight, room temperature

L6 ANSWER 5 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

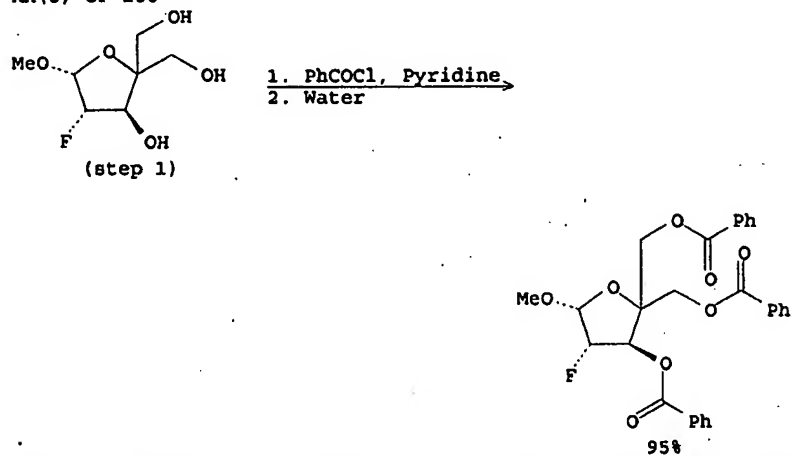
RX(8) OF 206



REF: Nucleosides, Nucleotides & Nucleic Acids, 20(4-7), 747-750;
2001
NOTE: stereoselective

L6 ANSWER 6 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

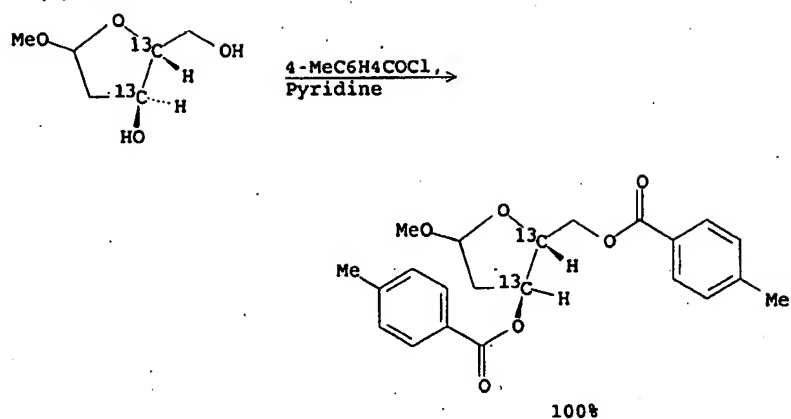
RX(8) OF 180



REF: Nucleosides, Nucleotides & Nucleic Acids, 20(8), 1583-1598;
2001

L6 ANSWER 7 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

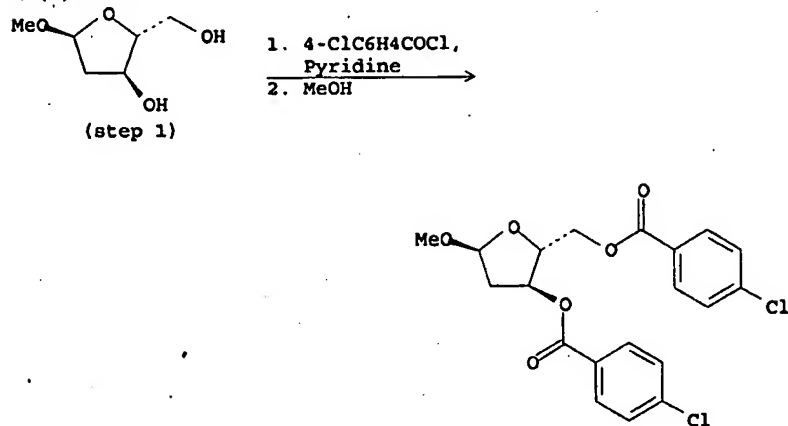
RX(9) OF 66



REF: European Journal of Organic Chemistry, (5), 861-866; 2000
CON: 2 hours, 40 deg C

L6 ANSWER 8 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

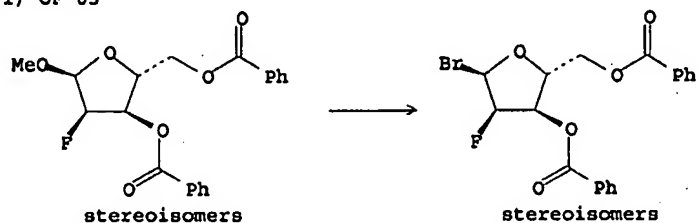
RX(6) OF 28



REF: Eur. Pat. Appl., 635517, 25 Jan 1995

L6 ANSWER 9 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

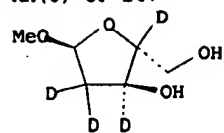
RX(1) OF 83



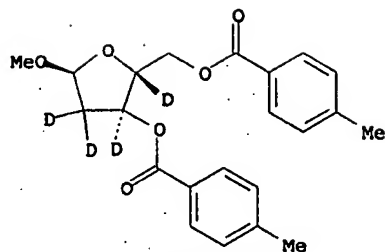
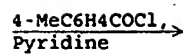
REF: PCT Int. Appl., 9310137, 27 May 1993
NOTE: 2 STEPS

L6 ANSWER 10 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(8) OF 147



stereoisomers

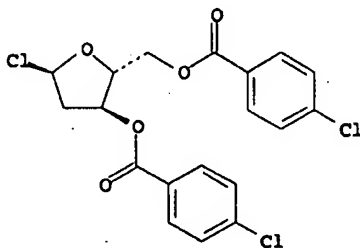
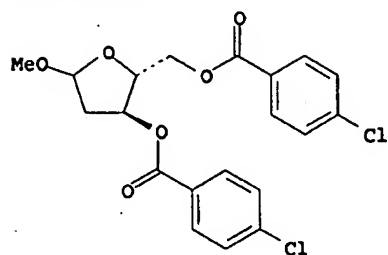


stereoisomers

REF: Tetrahedron, 43(18), 4227-34; 1987
NOTE: 87% overall

L6 ANSWER 11 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

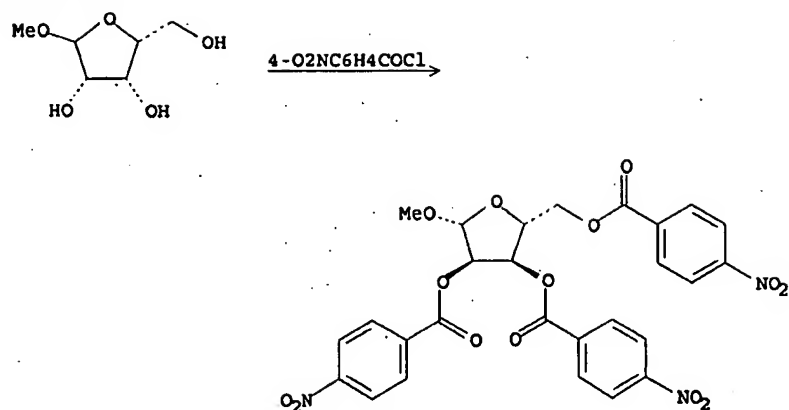
RX(2) OF 88



REF: Nippon Kagaku Kaishi, (12), 1765-70; 1986

L6 ANSWER 12 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

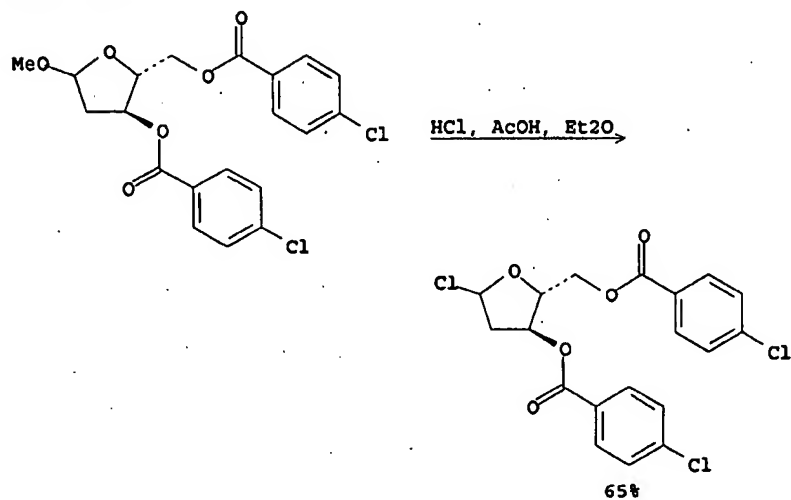
RX(1) OF 3



REF: U.S., 4282349, 04 Aug 1981

L6 ANSWER 13 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 13



REF: Journal of the American Chemical Society, 83,, 4066-50; 1961

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl
Et2O AcOH

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 18:00:49 ON 12 JUN 2007

SINCE FILE	TOTAL
ENTRY	SESSION
264.73	264.94

FILE 'CASREACT' ENTERED AT 15:44:56 ON 12 JUN 2007
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

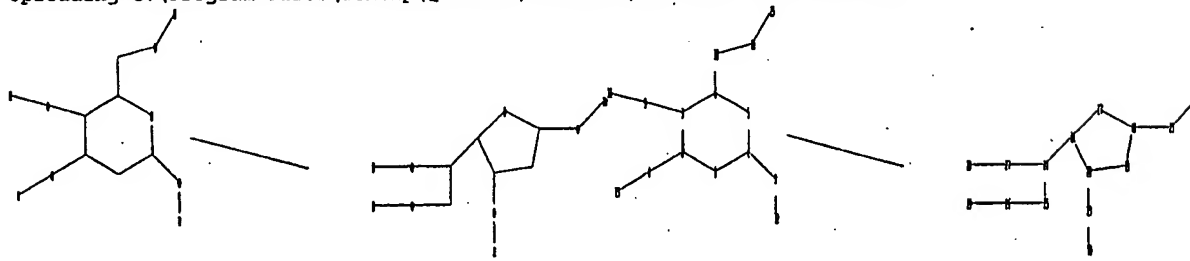
New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 12 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction II to III.str



chain nodes :
7 8 9 10 11 12 13 14 15 21 22 23 24 25 26 27 28 29 30
ring nodes :
1 2 3 4 5 6 16 17 18 19 20
chain bonds :
2-8 3-9 4-10 6-7 7-12 8-13 9-14 10-11 11-15 16-24 18-21 20-23 21-22 23-30 24-25 24-27
25-26 26-29 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 2-8 3-4 3-9 4-5 5-6 6-7 10-11 16-17 16-20 17-18 18-19 18-21 19-20 20-23
24-27 25-26
exact bonds :
4-10 7-12 8-13 9-14 11-15 16-24 21-22 23-30 24-25 26-29 27-28

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
fragments assigned product role:
containing 16
fragments assigned reactant/reagent role:
containing 1

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 15:45:15 FILE 'CASREACT'
SCREENING COMPLETE - 522 REACTIONS TO VERIFY FROM 17 DOCUMENTS

100.0% DONE 522 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 9070 TO 11810
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 15:45:23 FILE 'CASREACT'
SCREENING COMPLETE - 7531 REACTIONS TO VERIFY FROM 254 DOCUMENTS

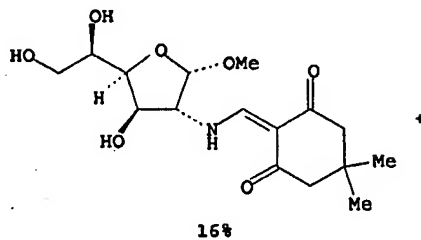
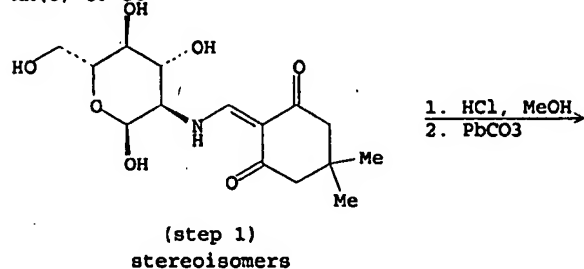
100.0% DONE 7531 VERIFIED 6 HIT RXNS 3 DOCS
SEARCH TIME: 00.00.02

L3 3 SEA SSS FUL L1 (6 REACTIONS)

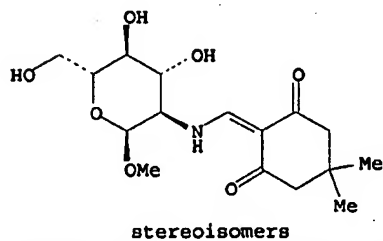
=> d l3 1-3

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(6) OF 56



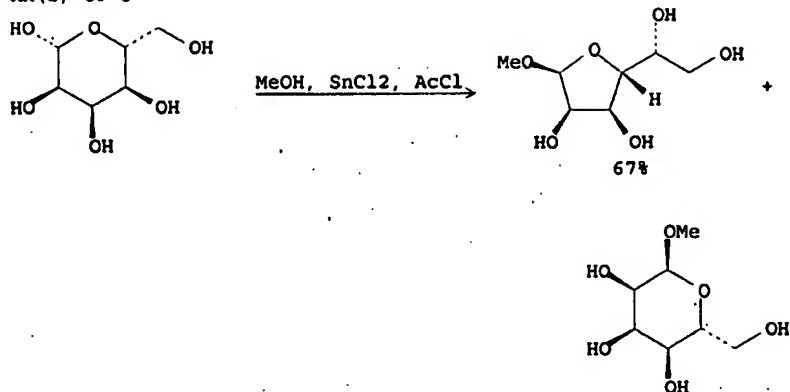
RX(6) OF 56



REF: Carbohydrate Research, 162(2), 181-97; 1987

L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 3

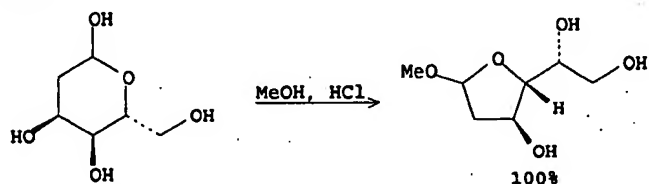


REF: Carbohydrate Research, 25(1), 43-8; 1972

NOTE: Classification: Heterocycle formation; Ring cleavage; Hydrolysis; Alkoxylation; # Conditions: SnCl₂ AcCl; Rf 200mm; # Comments: yield for alpha anomer of 5-membered ring. 14% yield for; beta anomer. 6% yield for alpha anomer of 6-membered ring; product. 8% yield for beta anomer

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1



REF: Chemical Communications (London), (14), 808-9; 1968

NOTE: Classification: Alkoxylation; Acetalisation; Ring contraction; # Conditions: MeOH HCl 6mm 20 deg; # Comments: alpha/beta=1/1 for product

=> d his

(FILE 'HOME' ENTERED AT 15:44:45 ON 12 JUN 2007)

FILE 'CASREACT' ENTERED AT 15:44:56 ON 12 JUN 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 3 S L1 FULL

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE
ENTRY
122.13

TOTAL
SESSION
122.34

STN INTERNATIONAL LOGOFF AT 15:45:46 ON 12 JUN 2007

FILE 'CASREACT' ENTERED AT 16:48:14 ON 12 JUN 2007
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

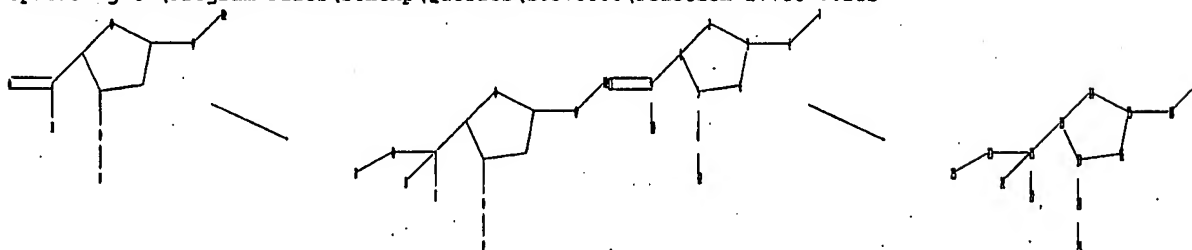
New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 12 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction iv.to v.str



chain nodes :
6 7 8 9 10 11 12 18 19 20 21 22 23 24 25 26
ring nodes :
1 2 3 4 5 13 14 15 16 17
chain bonds :
1-9 3-6 5-8 6-7 8-12 9-10 9-11 13-21 15-18 17-20 18-19 20-24 21-22 21-23 21-26 23-25
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 2-3 3-4 3-6 4-5 5-8 9-11 13-14 13-17 14-15 15-16 15-18 16-17 17-20 21-23
exact bonds :
1-9 6-7 8-12 9-10 13-21 18-19 20-24 21-22 21-26 23-25

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS
fragments assigned product role:
containing 13
fragments assigned reactant/reagent role:
containing 1

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s ;1
ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end
SEARCH ENDED BY USER

L2 407826 1

=> s l1
SAMPLE SEARCH INITIATED 16:48:44 FILE 'CASREACT'
SCREENING COMPLETE - 1397 REACTIONS TO VERIFY FROM 100 DOCUMENTS

100.0% DONE 1397 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 25700 TO 30180
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 16:48:49 FILE 'CASREACT'
SCREENING COMPLETE - 32058 REACTIONS TO VERIFY FROM 1917 DOCUMENTS

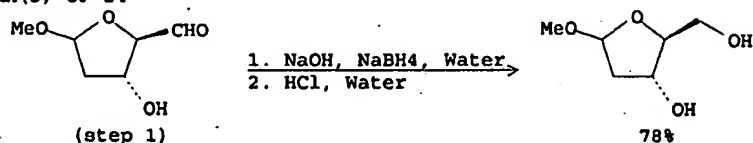
100.0% DONE 32058 VERIFIED 1 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.03

L4 1 SEA SSS FUL L1 (1 REACTIONS)

=> d l4

L4 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 24



REF: PCT Int. Appl., 2005044832, 19 May 2005
CON: STAGE(1) room temperature -> 0 deg C; <15 deg C; 30 minutes,
cooled
STAGE(2) pH 7

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

118.78

118.99

STN INTERNATIONAL LOGOFF AT 16:49:38 ON 12 JUN 2007

FILE 'CASREACT' ENTERED AT 16:44:50 ON 12 JUN 2007
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

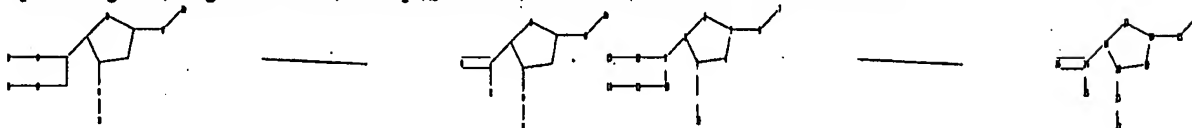
New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 12 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction III to IV.str



chain nodes :
6 7 8 9 10 11 12 13 14 15 21 22 23 24 25 26 27
ring nodes :
1 2 3 4 5 16 17 18 19 20
chain bonds :
1-9 3-6 5-8 6-7 8-15 9-10 9-12 10-11 11-14 12-13 16-24 18-21 20-23 21-22 23-27 24-25
24-26
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 2-3 3-4 3-6 4-5 5-8 9-12 10-11 16-17 16-20 17-18 18-19 18-21 19-20 20-23 24-26
exact bonds :
1-9 6-7 8-15 9-10 11-14 12-13 16-24 21-22 23-27 24-25

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS
fragments assigned product role:
containing 16

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 16:45:06 FILE 'CASREACT'
SCREENING COMPLETE - 375 REACTIONS TO VERIFY FROM 18 DOCUMENTS
100.0% DONE 375 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 6339 TO 8661
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 16:45:12 FILE 'CASREACT'

SCREENING COMPLETE - 7002 REACTIONS TO VERIFY FROM 321 DOCUMENTS

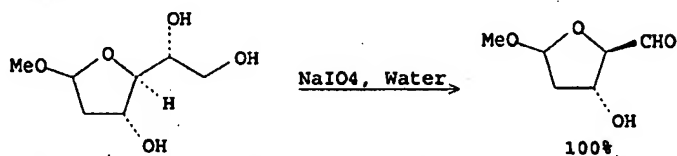
100.0% DONE 7002 VERIFIED 4 HIT RXNS 3 DOCS
SEARCH TIME: 00.00.05

L3 3 SEA SSS FUL L1 (4 REACTIONS)

=> d l3 1-3

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

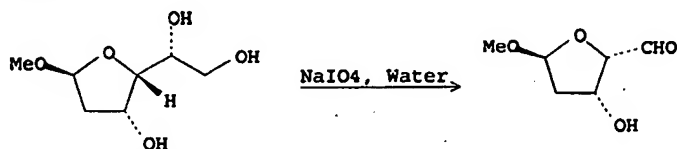
RX(2) OF 24



REF: PCT Int. Appl., 2005044832, 19 May 2005
CON: STAGE(1) <0 deg C; 30 minutes, <10 deg C

L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

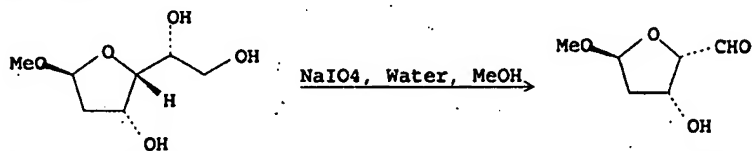
RX(2) OF 15



REF: Carbohydrate Research, 181,, 125-34; 1988

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 39



REF: Journal of the American Chemical Society, 107(18), 5283-5; 1985

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
122.13	122.34

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FILE LAST UPDATED: 11 Jun 2007 (20070611/ED)

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L4 3 L3

=> d 14 1-3 ibib hitstr

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:429422 CAPLUS
DOCUMENT NUMBER: 142:463961
TITLE: Process for the preparation of 1-chloro-3,5-di-O-acyl-
2-deoxy-L-ribofuranoside derivatives from
2-deoxy-D-galactose via stereoselective chlorination
reaction
INVENTOR(S): Tamerlani, Giancarlo; Bartalucci, Debora; Salsini,
Liana; Rapaccini, Silvia
PATENT ASSIGNEE(S): Inalco S.p.A., Italy
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005044832	A1	20050519	WO 2004-EP52900	20041110
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2545437	A1	20050519	CA 2004-2545437	20041110
EP 1699805	A1	20060913	EP 2004-818161	20041110
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS			
CN 1878782	A	20061213	CN 2004-80033026	20041110
JP 2007510696	T	20070426	JP 2006-538856	20041110
US 2007083041	A1	20070412	US 2006-578800	20060509
PRIORITY APPLN. INFO.:			IT 2003-FI288	A 20031110
			WO 2004-EP52900	W 20041110
OTHER SOURCE(S):	CASREACT 142:463961; MARPAT 142:463961			
REFERENCE COUNT:	1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT			

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:173573 CAPLUS
DOCUMENT NUMBER: 110:173573
TITLE: Synthesis of 2-deoxy-D-arabino-(6-13C)hexose
AUTHOR(S): Walker, Thomas E.; Ehler, Deborah S.; Unkefer, Clifford J.
CORPORATE SOURCE: Los Alamos Natl. Lab., Los Alamos, NM, 87545, USA
SOURCE: Carbohydrate Research (1988), 181, 125-34
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:173573

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:560278 CAPLUS
DOCUMENT NUMBER: 103:160278
TITLE: Total synthesis of the cytochrome P-450 epoxxygenase metabolites 5(R),6(S)-, 5(S),6(R)-, and 14(R),15(S)-epoxyeicosatrienoic acid (EET) and hydration products 5(R),6(R)- and 14(R),15(R)-dihydroxyeicosatrienoic acid (DHET)
AUTHOR(S): Moustakis, Christine A.; Viala, Jacques; Capdevila, Jorge; Falck, J. R.
CORPORATE SOURCE: Health Sci. Cent., Univ. Texas, Dallas, TX, 75235, USA
SOURCE: Journal of the American Chemical Society (1985), 107(18), 5283-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:160278

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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

4.01

126.35

STN INTERNATIONAL LOGOFF AT 16:46:12 ON 12 JUN 2007